# Author Index to Volume 147

Adamowicz, L., see E.R. Davidson	147 (1990) 45
Alberts, I.L., see Y. Yamaguchi	147 (1990) 309
Åman, C., J.B.C. Pettersson and L. Holmlid, Field ionizable cesium metal clusters from	
a foil diffusion source	147 (1990) 189
Angelov, S., see J. Degen	147 (1990) 415
Ascone, I., see C. Gauthier	147 (1990) 165
Atanasov, M., see J. Degen	147 (1990) 415
Barbe, JM., see C. Gauthier	147 (1990) 165
Barrett, J.C., see K. Leung	147 (1990) 257
Bauer, G., see N. Trendafilova	147 (1990) 377
Bednarová, L., see P. Pančoška	147 (1990) 401
Beijerinck, H.C.W., see J.P.J. Driessen	147 (1990) 447
Bijnen, F., see R. Fantoni	147 (1990) 389
Billing, G.D., A. Guldberg, N.E. Henriksen and F.Y. Hansen, Dissociative chemisorption	
of N <sub>2</sub> on rhenium: dynamics at low impact energies	147 (1990) 1
Bisht, P.B., H.B. Tripathi and D.D. Pant, Reinvestigation of the photophysics of the	
2-naphthol-amine hydrogen-bonded system. I	147 (1990) 173
Blöcker, J.H., EA. Reinsch, P. Rosmus, HJ. Werner and P.J. Knowles, Theoretical ra-	
diative transition probabilities of the CS <sup>+</sup> ion	147 (1990) 99
Bock, C.W., Y.N. Panchenko and S.V. Krasnoshchiokov, An ab initio vibrational study of	
rotational isomerism in oxalyl fluoride, O=CF-CF=O, and acryloyl fluoride, O=CF-	
CH=CH <sub>2</sub>	147 (1990) 65
Bogatchev, G., see N. Trendafilova	147 (1990) 377
Boyle, C.M., see E.R. Davidson	147 (1990) 45
Brion, C.E., see E.R. Davidson	147 (1990) 45
Brion, C.E., see K.H. Sze	147 (1990) 219
Buenker, R.J., see S. Roszak	147 (1990) 13
Buenker, R.J., see S.N. Rai	147 (1990) 327
Butz, T., see P. Mottner	147 (1990) 199
Carter, S., see J. Senekowitsch	147 (1990) 281
Chang, X.Y., see M.R. Hand	147 (1990) 351
Chesnut, D.B. and C.G. Phung, Functional counterpoise corrections for the NMR chemical shift in a model dimeria water system.	147 (1000) 01
ical shift in a model dimeric water system	147 (1990) 91
Clark, S.A.C., see E.R. Davidson	147 (1990) 45
Clotet, A., J.P. Daudey, J.P. Malrieu, J. Rubio and F. Spiegelmann, The effect of dynamical correlation on the valence wavefunction of molecules: dressed complete active space	
self-consistent field calculations	147 (1990) 293
Cortes, R., see C. Gauthier	147 (1990) 165

# Author Index to Volume 147

Adamowicz, L., see E.R. Davidson	147 (1990) 45
Alberts, I.L., see Y. Yamaguchi	147 (1990) 309
Åman, C., J.B.C. Pettersson and L. Holmlid, Field ionizable cesium metal clusters from	
a foil diffusion source	147 (1990) 189
Angelov, S., see J. Degen	147 (1990) 415
Ascone, I., see C. Gauthier	147 (1990) 165
Atanasov, M., see J. Degen	147 (1990) 415
Barbe, JM., see C. Gauthier	147 (1990) 165
Barrett, J.C., see K. Leung	147 (1990) 257
Bauer, G., see N. Trendafilova	147 (1990) 377
Bednarová, L., see P. Pančoška	147 (1990) 401
Beijerinck, H.C.W., see J.P.J. Driessen	147 (1990) 447
Bijnen, F., see R. Fantoni	147 (1990) 389
Billing, G.D., A. Guldberg, N.E. Henriksen and F.Y. Hansen, Dissociative chemisorption	
of N <sub>2</sub> on rhenium: dynamics at low impact energies	147 (1990) 1
Bisht, P.B., H.B. Tripathi and D.D. Pant, Reinvestigation of the photophysics of the	
2-naphthol-amine hydrogen-bonded system. I	147 (1990) 173
Blöcker, J.H., EA. Reinsch, P. Rosmus, HJ. Werner and P.J. Knowles, Theoretical ra-	
diative transition probabilities of the CS <sup>+</sup> ion	147 (1990) 99
Bock, C.W., Y.N. Panchenko and S.V. Krasnoshchiokov, An ab initio vibrational study of	
rotational isomerism in oxalyl fluoride, O=CF-CF=O, and acryloyl fluoride, O=CF-	
CH=CH <sub>2</sub>	147 (1990) 65
Bogatchev, G., see N. Trendafilova	147 (1990) 377
Boyle, C.M., see E.R. Davidson	147 (1990) 45
Brion, C.E., see E.R. Davidson	147 (1990) 45
Brion, C.E., see K.H. Sze	147 (1990) 219
Buenker, R.J., see S. Roszak	147 (1990) 13
Buenker, R.J., see S.N. Rai	147 (1990) 327
Butz, T., see P. Mottner	147 (1990) 199
Carter, S., see J. Senekowitsch	147 (1990) 281
Chang, X.Y., see M.R. Hand	147 (1990) 351
Chesnut, D.B. and C.G. Phung, Functional counterpoise corrections for the NMR chemical shift in a model dimeria water system.	147 (1000) 01
ical shift in a model dimeric water system	147 (1990) 91
Clark, S.A.C., see E.R. Davidson	147 (1990) 45
Clotet, A., J.P. Daudey, J.P. Malrieu, J. Rubio and F. Spiegelmann, The effect of dynamical correlation on the valence wavefunction of molecules: dressed complete active space	
self-consistent field calculations	147 (1990) 293
Cortes, R., see C. Gauthier	147 (1990) 165

Daudey, J.P., see A. Clotet	147 (1990) 293
Davidson, E.R., D. Feller, C.M. Boyle, L. Adamowicz, S.A.C. Clark and C.E. Brion, Har-	
tree-Fock limit and configuration interaction calculations of the ion-molecule overlap	
amplitude for hydrogen fluoride: comparison with EMS experiments	147 (1990) 45
Degen, J., HH. Schmidtke, R. Stoyanova, S. Angelov and M. Atanasov, Emission spectra	
of CO <sub>2</sub> radicals, stabilized in SrCO <sub>3</sub> obtained by thermal decomposition of SrC <sub>2</sub> O <sub>4</sub> ·H <sub>2</sub> O	147 (1990) 415
Driessen, J.P.J., H.J.L. Megens, M.J. Zonneveld, H.A.J. Senhorst, H.C.W. Beijerinck and	
B.J. Verhaar, Pure state Ne*(*) [ $ J, M\rangle$ ]-preparation in a magnetic field: polarization	
effects in ionizing collisions	147 (1990) 447
Drobny, G.P., see B. Ewing	147 (1990) 121
Duke, C.B., see J.P. LaFemina	147 (1990) 343
Enzo, S., see R. Fantoni	147 (1990) 389
Ewing, B., S.J. Glaser and G.P. Drobny, Development and optimization of shaped NMR	(,
pulses for the study of coupled spin systems	147 (1990) 121
panded for the stady of coupled opin systems	(1770) 121
Fantoni, R., F. Bijnen, S. Piccirillo and S. Enzo, Investigation of laser induced silane/hy-	
drocarbon reactions in the formation of Si and SiC powders	147 (1990) 389
Feller, D., see E.R. Davidson	147 (1990) 45
Fernandez Pacios, L., Valence electronic densities and electrostatic potentials in ab initio	147 (1990) 43
effective core potential procedures	147 (1000) 225
	147 (1990) 335 147 (1990) 241
Forst, W., On approximately exponential relaxation of polyatomics in bulk systems	147 (1990) 241
Fujii, T., K. Kakizaki and H. Ishii, Surface ionization of organometallic compounds: or-	147 (1000) 212
ganic derivatives of main group III-V elements	147 (1990) 213
Gauthier, C., I. Ascone, J. Goulon, R. Cortes, JM. Barbe and R. Guilard, First experi-	
mental evidence of circularly polarized X-ray excited optical luminescence (XEOL)	
from chiral Eu <sup>3+</sup> complexes	147 (1990) 165
Glaser, S.J., see B. Ewing	147 (1990) 103
Goddard, J.D., see Y. Yamaguchi	147 (1990) 121
Goez, M., Flash CIDNP investigation of a cyclic photoreaction	147 (1990) 143
Goulon, J., see C. Gauthier	147 (1990) 165
Grimm, F.A., see B.W. Yates	147 (1990) 431
Guest, M.F., see M.H. Palmer	147 (1990) 19
Guilard, R., see C. Gauthier	147 (1990) 165
Guldberg, A., see G.D. Billing	147 (1990) 1
Hand, M.R., X.Y. Chang and S. Holloway, A theoretical scattering study of oriented NO	
from a silver surface: effects of surface recoil	147 (1990) 351
Hansen, F.Y., see G.D. Billing	147 (1990) 1
Hanson, D.M., see H. Yang	147 (1990) 115
Hariharan, P.C., see S. Roszak	147 (1990) 13
Henriksen, N.E., see G.D. Billing	147 (1990) 1
Hitchcock, A.P., A.T. Wen and E. Rühl, Transition metal 2p excitation of organometallic	()
compounds studied by electron energy loss spectroscopy	147 (1990) 51
Holloway, S., see M.R. Hand	147 (1990) 351
Holmlid, L., see C. Åman	147 (1990) 189
Hommid, E., See C. Aman	147 (1990) 109

Hopkirk, A., see M.H. Palmer	147 (1990) 19
Huang, MB. and S. Lunell, Equilibrium structure and hyperfine parameters of the ethane	
cation	147 (1990) 85
Hurst, M., see R.W. Munn	147 (1990) 35
Ishii, H., see T. Fujii	147 (1990) 213
Ito, M., see H. Matsuzawa	147 (1990) 77
Iwata, S., see H. Matsuzawa	147 (1990) 77
Joachim, C., J.P. Launay and S. Woitellier, Distance dependence of the effective coupling	
parameters through conjugated ligands of the polyene type	147 (1990) 131
Jodl, H.J., see M. Jordan	147 (1990) 155
Johari, G.P., see D. Sidebottom	147 (1990) 205
Jordan, M., H.J. Jodl and M. Maier, High resolution Raman measurements of the tem-	(,
perature dependence of the phonon linewidth in lithium formate monohydrate crystals	147 (1990) 155
Kakizaki, K., see T. Fujii	147 (1990) 213
Kaufman, J.J., see S. Roszak	147 (1990) 13
Kellner, R., see N. Trendafilova	147 (1990) 377
Khoroshilov, E.V., see D.N. Nikogosyan	147 (1990) 437
Khoroshilova, E.V., see D.N. Nikogosyan	147 (1990) 437
Knierim, K.D., Hot atom kinetic theory: changes in average reaction energy	147 (1990) 109
Knowles, P.J., see J.H. Blöcker	147 (1990) 99
Král, M., see P. Pančoška	147 (1990) 401
Krasnoshchiokov, S.V., see C.W. Bock	147 (1990) 65
Kryukov, I.V., see D.N. Nikogosyan	147 (1990) 437
LaFemina, J.P., C.B. Duke and W. Rettig, Molecular conformations from ultraviolet	
photoelectron spectra: substituted anilines	147 (1990) 343
Launay, J.P., see C. Joachim	147 (1990) 131
Leung, K., J.C. Barrett and B. Shizgal, Thermal mobilities of electrons in binary rare gas	
mixtures	147 (1990) 257
Lunell, S., see MB. Huang	147 (1990) 85
Maier, M., see M. Jordan	147 (1990) 155
Maloň, P., see P. Pančoška	147 (1990) 401
Malrieu, J.P., see A. Clotet	147 (1990) 293
Matsuzawa, H., H. Yamashita, M. Ito and S. Iwata, Induced infrared absorption bands of ethylene adsorbed on mordenites: experimental and theoretical studies of electron-do-	
nor-acceptor interactions	147 (1990) 77
Megens, H.J.L., see J.P.J. Driessen	147 (1990) 447
Mikosch, H., see N. Trendafilova	147 (1990) 377
Mottner, P. and T. Butz, The nuclear quadrupole interaction of $^{187}W(\beta^-)^{187}Re$ in a 2H-	(.,,0, 3//
WS <sub>2</sub> single crystal	147 (1990) 199
Munn, R.W. and M. Hurst, Screened dipolar interactions in some molecular crystals	147 (1990) 35
and ha rates, servence dipolar interactions in some indicodular of ystais	147 (1770) 33

Nikogosyan, D.N., Yu.A. Repeyev, E.V. Khoroshilova, I.V. Kryukov, E.V. Khoroshilov and A.V. Sharkov, Asymmetric photolysis of biomolecules under high-intensity UV laser		
irradiation	147 (1990) 437	
Nikolov, G.St., see N. Trendafilova	147 (1990) 377	7
Nyeland, C., K.T. Tang and J.P. Toennies, Repulsive ion-atom and ion-ion potentials from		
charge density overlap integrals	147 (1990) 229	)
Palmer, M.H., I.C. Walker, M.F. Guest and A. Hopkirk, The electronic states of the azines. III. Pyrimidine, studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration calculations	147 (1990) 19	9
Panchenko, Y.N., see C.W. Bock	147 (1990) 6:	
Pančoška, P., M. Urbanová, L. Bednárová, K. Vacek, V.Z. Paschenko, S. Vasiliev, P. Maloň and M. Král, Models of pigment-protein interactions in photosynthetic systems: tetraphenylporphyrin complexes with polycationic sequential polypeptides. Absorption cir-		
cular dichroism and fluorescence properties	147 (1990) 40	
Pant, D.D., see P.B. Bisht	147 (1990) 17	
Paschenko, V.Z., see P. Pančoška	147 (1990) 40	
Pettersson, J.B.C., see C. Åman	147 (1990) 18	
Phillips, D., see E. Vauthey	147 (1990) 42	
Phung, C.G., see D.B. Chesnut	147 (1990) 9	
Piccirillo, S., see R. Fantoni	147 (1990) 38	9
Rai, S.N. and R.J. Buenker, Theoretical prediction of the radiative lifetimes of the two		
lowest excited electronic states of TeO	147 (1990) 32	!7
Rashev, S., Anharmonic interactions and intramolecular vibrational energy redistribution		
in anthracene	147 (1990) 22	
Reinsch, EA., see J.H. Blöcker	147 (1990) 9	
Repeyev, Yu.A., see D.N. Nikogosyan	147 (1990) 43	
Rettig, W., see J.P. LaFemina	147 (1990) 34	
Rosmus, P., see J.H. Blöcker	147 (1990) 9	
Rosmus, P., see J. Senekowitsch	147 (1990) 28	31
Roszak, S., R.J. Buenker, P.C. Hariharan and J.J. Kaufman, Ab intio MRD CI ground and excited state potential curves for addition of O to H <sub>2</sub> C=CH <sub>2</sub> and oxirane formation and		
decomposition	147 (1990)	
Rubio, J., see A. Clotet	147 (1990) 29	
Rühl, E., see A.P. Hitchcock	147 (1990)	51
Schaefer III, H.F., see Y. Yamaguchi	147 (1990) 30	09
Schmidtke, HH., see J. Degen	147 (1990) 4	15
Senekowitsch, J., S. Carter, P. Rosmus and HJ. Werner, Potential energy and dipole mo-		
ment functions of the HCS radical	147 (1990) 28	81
Senhorst, H.A.J., see J.P.J. Driessen	147 (1990) 4	47
Sharkov, A.V., see D.N. Nikogosyan	147 (1990) 43	37
Shizgal, B., see K. Leung	147 (1990) 2:	57
Shizgal, B., Negative differential conductivity of electrons in He-Xe and He-Kr mixtures Shkrob, I.A. and V.F. Tarasov, Magnetic field and magnetic isotope effects in micelles. The	147 (1990) 2	71
kinetics of photochemical reactions	147 (1990) 3	69

Sidebottom, D. and G.P. Johari, Chemical and physical effects during spontaneous relax-	
ation of a network-structure glass	147 (1990) 205
Spiegelmann, F., see A. Clotet	147 (1990) 293
Stoyanova, R., see J. Degen	147 (1990) 415
Sze, K.H. and C.E. Brion, Inner-shell and valence-shell electronic excitation of SF <sub>6</sub> , SeF <sub>6</sub>	
and TeF <sub>6</sub> by high energy electron impact: an investigation of potential barrier effects.	
Chem. Phys. 140 (1990) 439. Erratum	147 (1990) 219
Tang, K.T., see C. Nyeland	147 (1990) 229
Tarasov, V.F., see I.A. Shkrob	147 (1990) 369
Taylor, J.W., see B.W. Yates	147 (1990) 431
Toennies, J.P., see C. Nyeland	147 (1990) 229
Trendafilova, N., G.St. Nikolov, R. Kellner, H. Mikosch, G. Bauer and G. Bogatchev, Manifestation of the Jahn-Teller active vibrations in the vibronic spectra of tetra-	
coordinate Cu <sup>2+</sup> , Ni <sup>2+</sup> and Zn <sup>2+</sup> chlorides	147 (1990) 377
Trentini, F.V., see H. Yang	147 (1990) 115
Tripathi, H.B., see P.B. Bisht	147 (1990) 173
Tse, J.S., see B.W. Yates	147 (1990) 431
Urbanová, M., see P. Pančoška	147 (1990) 401
Vacek, K., see P. Pančoška	147 (1990) 401
Vasiliev, S., see P. Pančoška	147 (1990) 401
Vauthey, E. and D. Phillips, Viscosity effect on the rate of back electron transfer within	
a short-lived exciplex	147 (1990) 421
Verhaar, B.J., see J.P.J. Driessen	147 (1990) 447
Von Wald, G.A., see B.W. Yates	147 (1990) 431
Walker, I.C., see M.H. Palmer	147 (1990) 19
Wen, A.T., see A.P. Hitchcock	147 (1990) 51
Werner, HJ., see J.H. Blöcker	147 (1990) 99
Werner, HJ., see J. Senekowitsch	147 (1990) 281
Whitten, J.L., see H. Yang	147 (1990) 115
Woitellier, S., see C. Joachim	147 (1990) 131
Yamaguchi, Y., I.L. Alberts, J.D. Goddard and H.F. Schaefer III, Use of the molecular or-	
bital Hessian for self-consistent-field (SCF) wavefunctions	147 (1990) 309
Yamashita, H., see H. Matsuzawa	147 (1990) 77
Yang, H., D.M. Hanson, F.V. Trentini and J.L. Whitten, Multiparent configuration inter- action calculations of low-lying states of O <sub>2</sub> <sup>2+</sup>	147 (1990) 115
Yates, B.W., G.A. von Wald, J.W. Taylor, F.A. Grimm and J.S. Tse, Angle-resolved photo-	. 17 (1770) 113
electron study of the group VIB metal hexacarbonyls M(CO) <sub>6</sub> (M=Cr, Mo, W) from	
9 to 30 eV photon energy	147 (1990) 431
	(/
Zonneveld, M.J., see J.P.J. Driessen	147 (1990) 447

## List of Subjects

#### 1 Methods

#### 1.1 Theoretical

- 1.1.1 Group theory and algebras
- 1.1.2 Classical mechanics \*
- 1.1.3 Quantized field theory
- 1.1.4 Many body and quasiparticle approaches \*
- 1.1.5 Coupling schemes and perturbative treatments \*
- 1.1.6 Relativistic quantum mechanics
- 1.1.7 Transport quantum mechanics \*
- Equilibrium statistical mechanics \* 1.1.8
- 1.1.9 Statistical mechanics of stationary states
- Non-equilibrium thermodynamic and hydrodynamic 1.1.10 theories \*
- 1.1.11 Ab initio schemes for stationary properties \*
- 1.1.12 Computational and simulation methods \*
- 1.1.13 Molecular dynamics and scattering theory \*

#### 1.2 Experimental

- Magnetic resonances \* 1.2.1
- 1.2.2 Cyclotron resonance
- 1.2.3 Microwave spectroscopy
- 1.2.4 Infrared spectroscopy \*
- 1.2.5 Raman spectroscopy \*
- 1.2.6 Visible and UV spectroscopy \*
- 1.2.7 Fluorescence spectroscopy 4
- 1.2.8 Photoelectron and Auger spectroscopy \*
- X-ray spectroscopy \* 1.2.9
- 1.2.10 Electron impact spectroscopy \*
- 1.2.11 Laser methods \*
- 1.2.12 Picosecond spectroscopy \*
- Non-linear optical spectroscopy \* 1.2.13
- 1.2.14 Synchrotron spectroscopies
- 1.2.15 Coherent optical spectroscopy
- 1.2.16 Optical pumping \*
- 1.2.17 Multiple resonance spectroscopy
- 1.2.18 Optoacoustic spectroscopy
- 1.2.19 Atomic and molecular beam techniques \*
- 1.2.20 Time-resolved experiments \*
- 1.2.21 Mass spectrometry \*
- 1.2.22 Radiolysis
- 1.2.23 Mössbauer spectroscopy
- 1.2.24 X-ray, electron and neutron diffraction
- 1.2.25 Neutron scattering
- 1.2.26 Light scattering
- 1.2.27 Field emission and field ionization
- 1.2.28 Measurement of macroscopic variables

#### 2 Objects

#### 2.1 Bulk systems

- 2.1.1 Gases \*
- 2.1.2 Supersonic beams \*
- 2.1.3 Liquids neat
- 2.1.4 Liquid mixtures and solutions \*
- 2.1.5 Crystals \*
- 2.1.5.1 neat
- 2.1.5.2 mixed \*
- Glasses \* 2.1.6
- 2.1.7 Liquid crystals \*
- 2.1.8 Polymers \*
- 2.1.9 Semiconductors
- Metals and alloys 2.1.10
- 2.1.11 Thin films
- 2.1.12 Surfaces \*
- 2.1.13 Low-dimensional materials
- 2.1.14 Dielectrics \*
- 2.1.15 Plasmas
- 2.1.16 Biological systems

#### 2.2 Microscopic systems

- 2.2.1 Atoms \*
- 2.2.2 Molecules (neutral and ionic) \*
- 2.2.2.1 diatomic \*
- 2.2.2.2 small polyatomics \*
- 2.2.2.3 aromatics \*
- 2.2.2.4 other large
- 2.2.2.5 polymeric and biological \*
- 2.2.3 Molecular aggregates \*
- 2.2.3.1 dimers \*
- van der Waals molecules 2.2.3.2
- 2.2.3.3 clusters \*
- 2.2.3.4 complexes \*
- 2.2.4 Free radicals (including hydronium and muonium) \*
- 2.2.5 Quasiparticles (including excitons)
- 2.2.6 Defects and impurities
- 2.2.7 Ions and charge carriers \*

<sup>\*</sup> Denotes subjects covered in this volume

#### 3 Phenomena

		3.16	Multiphoton phenomena *
3.1	Molecular structure *	3.17	Reactions (including dissociation) *
3.2	Vibrations and rotations of molecules *	3.17.1	gas phase *
3.3	Electronic structure and states *	3.17.2	condensed phase
3.4	Electric and magnetic properties *	3.17.3	photochemical *
3.5	Spin splittings *	3.18	Tunnelling *
3.6	Optical activity *	3.19	Electron transfer *
3.7	Molecular interactions *	3.20	Positron annihilation
3.8	Spectral bandshapes and intensities *	3.21	Ionization (including Rydberg states) *
3.9	Coupling of electronic and nuclear motion *	3.22	Molecular motion (including diffusive) *
3.10	Energy transfer processes *	3.23	Isotopic effects
3.11	Molecular photophysical processes *	3.24	Fluctuations and noise
3.12	Intramolecular dynamics *	3.25	Collective motion and excitations
3.12.1	radiationless transitions	3.26	Surface effects and catalysis *
3.12.2	vibrational energy redistribution (including	3.27	Thermodynamic and transport properties
	vibrational dissociation) *	3.28	Structure of solids and liquids *
3.13	Luminescence spectra, yields and lifetimes *	3.29	Critical phenomena
3.14	Coherence loss processes	3.30	Phase transitions
3.15	Non-linear responses (including optical)		

# Subject Index to Volume 147

## Methods

## Theoretical

Classical mechanics	
Screened dipolar interactions in some molecular crystals, R.W. Munn and M. Hurst	147 (1990) 35
Many body and quasiparticle approaches	
Hartree-Fock limit and configuration interaction calculations of the ion-molecule overlap amplitude for hydrogen fluoride: comparison with EMS experiments, E.R. Davidson,	
D. Feller, C.M. Boyle, L. Adamowicz, S.A.C. Clark and C.E. Brion	147 (1990) 45
Coupling schemes and perturbative treatments	
Anharmonic interactions and intramolecular vibrational energy redistribution in anthracene, S. Rashev	147 (1990) 221
Repulsive ion-atom and ion-ion potentials from charge density overlap integrals,	
C. Nyeland, K.T. Tang and J.P. Toennies	147 (1990) 229
Transport quantum mechanics	
Hartree-Fock limit and configuration interaction calculations of the ion-molecule overlap amplitude for hydrogen fluoride: comparison with EMS experiments, E.R. Davidson,	
D. Feller, C.M. Boyle, L. Adamowicz, S.A.C. Clark and C.E. Brion	147 (1990) 45
Equilibrium statistical mechanics	
On approximately exponential relaxation of polyatomics in bulk systems, W. Forst	147 (1990) 241
Non-equilibrium thermodynamic and hydrodynamic theories	
On approximately exponential relaxation of polyatomics in bulk systems, W. Forst	147 (1990) 241
Thermal mobilities of electrons in binary rare gas mixtures, K. Leung, J.C. Barrett and B. Shizgal	147 (1990) 257
Negative differential conductivity of electrons in He-Xe and He-Kr mixtures, B. Shizgal	147 (1990) 237
	(, (,
Ab initio schemes for stationary properties	
Ab intio MRD CI ground and excited state potential curves for addition of O to H <sub>2</sub> C=CH <sub>2</sub> and oxirane formation and decomposition, S. Roszak, R.J. Buenker, P.C. Hariharan and	
J.J. Kaufman	147 (1990) 13
The electronic states of the azines. III. Pyrimidine, studied by VUV absorption, near- threshold electron energy-loss spectroscopy and ab initio multi-reference configuration	
calculations, M.H. Palmer, I.C. Walker, M.F. Guest and A. Hopkirk	147 (1990) 19

An ab initio vibrational study of rotational isomerism in oxalyl fluoride, O=CF-CF=O, and acryloyl fluoride, O=CF-CH=CH <sub>2</sub> , C.W. Bock, Y.N. Panchenko and	147 (1000)	
S.V. Krasnoshchiokov Induced infrared absorption bands of ethylene adsorbed on mordenites: experimental and	147 (1990) 6	13
theoretical studies of electron-donor-acceptor interactions, H. Matsuzawa, H. Yamashita, M. Ito and S. Iwata	147 (1990) 7	17
Equilibrium structure and hyperfine parameters of the ethane cation, MB. Huang and S. Lunell	147 (1990) 8	35
Functional counterpoise corrections for the NMR chemical shift in a model dimeric water system, D.B. Chesnut and C.G. Phung	147 (1990) 9	)1
Theoretical radiative transition probabilities of the CS <sup>+</sup> ion, J.H. Blöcker, EA. Reinsch, P. Rosmus, HJ. Werner and P.J. Knowles	147 (1990) 9	99
Potential energy and dipole moment functions of the HCS radical, J. Senekowitsch,	, , , ,	
S. Carter, P. Rosmus and HJ. Werner  The effect of dynamical correlation on the valence wavefunction of molecules: dressed complete active space self-consistent field calculations, A. Clotet, J.P. Daudey,	147 (1990) 28	) [
J.P. Malrieu, J. Rubio and F. Spiegelmann Use of the molecular orbital Hessian for self-consistent-field (SCF) wavefunctions,	147 (1990) 29	)3
Y. Yamaguchi, I.L. Alberts, J.D. Goddard and H.F. Schaefer III	147 (1990) 30	)9
Theoretical prediction of the radiative lifetimes of the two lowest excited electronic states of TeO, S.N. Rai and R.J. Buenker	147 (1990) 32	27
Valence electronic densities and electrostatic potentials in ab initio effective core potential procedures, L. Fernandez Pacios	147 (1990) 33	35
Computational and simulation methods		
Functional counterpoise corrections for the NMR chemical shift in a model dimeric water system, D.B. Chesnut and C.G. Phung	147 (1990) 9	91
Theoretical radiative transition probabilities of the CS <sup>+</sup> ion, J.H. Blöcker, EA. Reinsch, P. Rosmus, HJ. Werner and P.J. Knowles	147 (1990) 9	99
Hot atom kinetic theory: changes in average reaction energy, K.D. Knierim	147 (1990) 10	
Multiparent configuration interaction calculations of low-lying states of O <sub>2</sub> <sup>2+</sup> , H. Yang,		
D.M. Hanson, F.V. Trentini and J.L. Whitten  Development and optimization of shaped NMR pulses for the study of coupled spin sys-	147 (1990) 11	
tems, B. Ewing, S.J. Glaser and G.P. Drobny Valence electronic densities and electrostatic potentials in ab initio effective core potential	147 (1990) 12	21
procedures, L. Fernandez Pacios  Molecular conformations from ultraviolet photoelectron spectra: substituted anilines,	147 (1990) 33	35
J.P. LaFemina, C.B. Duke and W. Rettig  A theoretical scattering study of oriented NO from a silver surface: effects of surface recoil,	147 (1990) 34	43
M.R. Hand, X.Y. Chang and S. Holloway	147 (1990) 35	51
Molecular dynamics and scattering theory		
Dissociative chemisorption of N <sub>2</sub> on rhenium: dynamics at low impact energies, G.D. Billing, A. Guldberg, N.E. Henriksen and F.Y. Hansen	147 (1990)	1
Distance dependence of the effective coupling parameters through conjugated ligands of the polyene type, C. Joachim, J.P. Launay and S. Woitellier	147 (1990) 13	31
Repulsive ion-atom and ion-ion potentials from charge density overlap integrals, C. Nyeland, K.T. Tang and J.P. Toennies	147 (1990) 2	
	()	_,

A theoretical scattering study of oriented NO from a silver surface: effects of surface recoil, M.R. Hand, X.Y. Chang and S. Holloway	147 (1990) 351
Experimental	
Magnetic resonances	
Development and optimization of shaped NMR pulses for the study of coupled spin systems, B. Ewing, S.J. Glaser and G.P. Drobny	147 (1990) 121
Flash CIDNP investigation of a cyclic photoreaction, M. Goez	147 (1990) 143
Infrared spectroscopy	
An ab initio vibrational study of rotational isomerism in oxalyl fluoride, O=CF-CF=O, and acryloyl fluoride, O=CF-CH=CH <sub>2</sub> , C.W. Bock, Y.N. Panchenko and	
S.V. Krasnoshchiokov  Induced infrared absorption bands of ethylene adsorbed on mordenites: experimental and	147 (1990) 65
theoretical studies of electron-donor-acceptor interactions, H. Matsuzawa,	
H. Yamashita, M. Ito and S. Iwata  Potential energy and dipole moment functions of the HCS radical, J. Senekowitsch,	147 (1990) 77
S. Carter, P. Rosmus and HJ. Werner	147 (1990) 281
Manifestation of the Jahn-Teller active vibrations in the vibronic spectra of tetracoor-	
dinate Cu <sup>2+</sup> , Ni <sup>2+</sup> and Zn <sup>2+</sup> chlorides, N. Trendafilova, G.St. Nikolov, R. Kellner, H. Mikosch, G. Bauer and G. Bogatchev	147 (1990) 377
Raman spectroscopy	
An ab initio vibrational study of rotational isomerism in oxalyl fluoride, O=CF-CF=O,	
and acryloyl fluoride, O=CF-CH=CH <sub>2</sub> , C.W. Bock, Y.N. Panchenko and	147 (1990) 65
S.V. Krasnoshchiokov  High resolution Raman measurements of the temperature dependence of the phonon line-	147 (1990) 63
width in lithium formate monohydrate crystals, M. Jordan, H.J. Jodl and M. Maier	147 (1990) 155
Manifestation of the Jahn-Teller active vibrations in the vibronic spectra of tetracoordinate Cu <sup>2+</sup> , Ni <sup>2+</sup> and Zn <sup>2+</sup> chlorides, N. Trendafilova, G.St. Nikolov, R. Kellner,	
H. Mikosch, G. Bauer and G. Bogatchev	147 (1990) 377
Investigation of laser induced silane/hydrocarbon reactions in the formation of Si and SiC	
powders, R. Fantoni, F. Bijnen, S. Piccirillo and S. Enzo	147 (1990) 389
Visible and UV spectroscopy	
The electronic states of the azines. III. Pyrimidine, studied by VUV absorption, near- threshold electron energy-loss spectroscopy and ab initio multi-reference configuration	
calculations, M.H. Palmer, I.C. Walker, M.F. Guest and A. Hopkirk	147 (1990) 19
Theoretical radiative transition probabilities of the CS+ ion, J.H. Blöcker, EA. Reinsch,	
P. Rosmus, HJ. Werner and P.J. Knowles  Distance dependence of the effective coupling parameters through conjugated ligands of	147 (1990) 99
the polyene type, C. Joachim, J.P. Launay and S. Woitellier	147 (1990) 131
First experimental evidence of circularly polarized X-ray excited optical luminescence	
(XEOL) from chiral Eu <sup>3+</sup> complexes, C. Gauthier, I. Ascone, J. Goulon, R. Cortes, J	147 (1990) 165
M. Barbe and R. Guilard  Reinvestigation of the photophysics of the 2-naphthol-amine hydrogen-bonded system. I,	147 (1990) 103
P.B. Bisht, H.B. Tripathi and D.D. Pant	147 (1990) 173

Molecular conformations from ultraviolet photoelectron spectra: substituted anilines, J.P. LaFemina, C.B. Duke and W. Rettig	147 (1990) 343
Models of pigment-protein interactions in photosynthetic systems: tetraphenylporphyrin complexes with polycationic sequential polypeptides. Absorption circular dichroism and fluorescence properties, P. Pančoška, M. Urbanová, L. Bednárová, K. Vacek,	, , , , , , , , , , , , , , , , , , , ,
V.Z. Paschenko, S. Vasiliev, P. Maloň and M. Král	147 (1990) 401
Fluorescence spectroscopy	
Theoretical radiative transition probabilities of the CS <sup>+</sup> ion, J.H. Blöcker, EA. Reinsch, P. Rosmus, HJ. Werner and P.J. Knowles	147 (1990) 99
First experimental evidence of circularly polarized X-ray excited optical luminescence (XEOL) from chiral Eu <sup>3+</sup> complexes, C. Gauthier, I. Ascone, J. Goulon, R. Cortes,	
JM. Barbe and R. Guilard	147 (1990) 165
Models of pigment-protein interactions in photosynthetic systems: tetraphenylporphyrin complexes with polycationic sequential polypeptides. Absorption circular dichroism and fluorescence properties, P. Pančoška, M. Urbanová, L. Bednárová, K. Vacek,	
V.Z. Paschenko, S. Vasiliev, P. Maloň and M. Král	147 (1990) 401
Emission spectra of CO <sub>2</sub> radicals, stabilized in SrCO <sub>3</sub> obtained by thermal decomposition	
of SrC <sub>2</sub> O <sub>4</sub> ·H <sub>2</sub> O, J. Degen, HH. Schmidtke, R. Stoyanova, S. Angelov and M. Atanasov	147 (1990) 415
Viscosity effect on the rate of back electron transfer within a short-lived exciplex, E. Vauthey and D. Phillips	147 (1990) 421
Photoelectron and Auger spectroscopy	
The electronic states of the azines. III. Pyrimidine, studied by VUV absorption, near- threshold electron energy-loss spectroscopy and ab initio multi-reference configuration	
calculations, M.H. Palmer, I.C. Walker, M.F. Guest and A. Hopkirk Molecular conformations from ultraviolet photoelectron spectra: substituted anilines,	147 (1990) 19
J.P. LaFemina, C.B. Duke and W. Rettig	147 (1990) 343
Angle-resolved photoelectron study of the group VIB metal hexacarbonyls M(CO) <sub>6</sub>	
(M=Cr, Mo, W) from 9 to 30 eV photon energy, B.W. Yates, G.A. von Wald, J.W. Taylor, F.A. Grimm and J.S. Tse	147 (1990) 431
X-ray spectroscopy	
Transition metal 2p excitation of organometallic compounds studied by electron energy loss spectroscopy, A.P. Hitchcock, A.T. Wen and E. Rühl	147 (1990) 51
First experimental evidence of circularly polarized X-ray excited optical luminescence (XEOL) from chiral Eu <sup>3+</sup> complexes, C. Gauthier, I. Ascone, J. Goulon, R. Cortes,	(,
JM. Barbe and R. Guilard	147 (1990) 165
Electron impact spectroscopy	
Hartree-Fock limit and configuration interaction calculations of the ion-molecule overlap amplitude for hydrogen fluoride: comparison with EMS experiments, E.R. Davidson,	
D. Feller, C.M. Boyle, L. Adamowicz, S.A.C. Clark and C.E. Brion	147 (1990) 45
Transition metal 2p excitation of organometallic compounds studied by electron energy	
loss spectroscopy, A.P. Hitchcock, A.T. Wen and E. Rühl	147 (1990) 51

Laser methods	
Flash CIDNP investigation of a cyclic photoreaction, M. Goez	147 (1990) 143
Picosecond spectroscopy	
Asymmetric photolysis of biomolecules under high-intensity UV laser irradiation, D.N. Nikogosyan, Yu.A. Repeyev, E.V. Khoroshilova, I.V. Kryukov, E.V. Khoroshilov and A.V. Sharkov	147 (1990) 437
Non-linear optical spectroscopy	
Investigation of laser induced silane/hydrocarbon reactions in the formation of Si and SiC powders, R. Fantoni, F. Bijnen, S. Piccirillo and S. Enzo	147 (1990) 389
Optical pumping	
Pure state $Ne^{*(*)}[ J,M\rangle]$ -preparation in a magnetic field: polarization effects in ionizing collisions, J.P.J. Driessen, H.J.L. Megens, M.J. Zonneveld, H.A.J. Senhorst, H.C.W. Beijerinck and B.J. Verhaar	147 (1990) 447
Atomic and molecular beam techniques	
Field ionizable cesium metal clusters from a foil diffusion source, C. Aman, J.B.C. Pettersson and L. Holmlid  Pure state $Ne^{*(*)}[ J,M\rangle$ ]-preparation in a magnetic field: polarization effects in ionizing	147 (1990) 189
collisions, J.P.J. Driessen, H.J.L. Megens, M.J. Zonneveld, H.A.J. Senhorst, H.C.W. Beijerinck and B.J. Verhaar	147 (1990) 447
Time-resolved experiments	
Flash CIDNP investigation of a cyclic photoreaction, M. Goez Reinvestigation of the photophysics of the 2-naphthol-amine hydrogen-bonded system. I,	147 (1990) 143
P.B. Bisht, H.B. Tripathi and D.D. Pant Field ionizable cesium metal clusters from a foil diffusion source, C. Åman,	147 (1990) 173
J.B.C. Pettersson and L. Holmlid	147 (1990) 189
The nuclear quadrupole interaction of $^{187}W(\beta^-)^{187}Re$ in a $2H-WS_2$ single crystal, P. Mottner and T. Butz	147 (1990) 199
Models of pigment-protein interactions in photosynthetic systems: tetraphenylporphyrin complexes with polycationic sequential polypeptides. Absorption circular dichroism and fluorescence properties, P. Pančoška, M. Urbanová, L. Bednárová, K. Vacek,	(,
V.Z. Paschenko, S. Vasiliev, P. Maloň and M. Král	147 (1990) 401
Emission spectra of CO <sub>2</sub> <sup>-</sup> radicals, stabilized in SrCO <sub>3</sub> obtained by thermal decomposition of SrC <sub>2</sub> O <sub>4</sub> ·H <sub>2</sub> O, J. Degen, HH. Schmidtke, R. Stoyanova, S. Angelov and M. Atanasov	147 (1990) 415
Viscosity effect on the rate of back electron transfer within a short-lived exciplex, E. Vauthey and D. Phillips	147 (1990) 421
Mass spectrometry	
Field ionizable cesium metal clusters from a foil diffusion source, C. Åman,	147 (1000) 100
J.B.C. Pettersson and L. Holmlid  Surface ionization of organometallic compounds: organic derivatives of main group III-	147 (1990) 189
V elements, T. Fujii, K. Kakizaki and H. Ishii	147 (1990) 213

## **Objects**

### **Bulk systems**

Gases	
Dissociative chemisorption of N <sub>2</sub> on rhenium: dynamics at low impact energies,	
G.D. Billing, A. Guldberg, N.E. Henriksen and F.Y. Hansen	147 (1990) 1
Hot atom kinetic theory: changes in average reaction energy, K.D. Knierim	147 (1990) 109
On approximately exponential relaxation of polyatomics in bulk systems, W. Forst	147 (1990) 241
Thermal mobilities of electrons in binary rare gas mixtures, K. Leung, J.C. Barrett and	147 (1000) 267
B. Shizgal	147 (1990) 257 147 (1990) 271
Negative differential conductivity of electrons in He-Xe and He-Kr mixtures, B. Shizgal	147 (1990) 271
Supersonic beams	
Anharmonic interactions and intramolecular vibrational energy redistribution in anthra-	
cene, S. Rashev	147 (1990) 221
Liquid mixtures and solutions	
Magnetic field and magnetic isotope effects in micelles. The kinetics of photochemical re-	
actions, I.A. Shkrob and V.F. Tarasov	147 (1990) 369
Viscosity effect on the rate of back electron transfer within a short-lived exciplex, E. Vauthey	
and D. Phillips	147 (1990) 421
Asymmetric photolysis of biomolecules under high-intensity UV laser irradiation,	
D.N. Nikogosyan, Yu.A. Repeyev, E.V. Khoroshilova, I.V. Kryukov, E.V. Khoroshilov	. 45 (1000) 435
and A.V. Sharkov	147 (1990) 437
Crystals	
Screened dipolar interactions in some molecular crystals, R.W. Munn and M. Hurst	147 (1990) 35
The nuclear quadrupole interaction of $^{187}W(\beta^-)^{187}Re$ in a $2H-WS_2$ single crystal,	
P. Mottner and T. Butz	147 (1990) 199
-mixed	
Manifestation of the Jahn-Teller active vibrations in the vibronic spectra of tetracoor-	
dinate Cu2+, Ni2+ and Zn2+ chlorides, N. Trendafilova, G.St. Nikolov, R. Kellner,	
H. Mikosch, G. Bauer and G. Bogatchev	147 (1990) 377
Glasses	
Chemical and physical effects during spontaneous relaxation of a network-structure glass,	
D. Sidebottom and G.P. Johari	147 (1990) 205
Liquid crystals	
Development and optimization of shaped NMR pulses for the study of coupled spin sys-	
tems, B. Ewing, S.J. Glaser and G.P. Drobny	147 (1990) 121
Polymers	
Chemical and physical effects during spontaneous relaxation of a network-structure glass,	
D. Sidebottom and G.P. Johari	147 (1990) 205

Surfaces		
Dissociative chemisorption of N <sub>2</sub> on rhenium: dynamics at low impact energies,		
G.D. Billing, A. Guldberg, N.E. Henriksen and F.Y. Hansen	147 (1990)	1
A theoretical scattering study of oriented NO from a silver surface: effects of surface recoil,	147 (1000)	
M.R. Hand, X.Y. Chang and S. Holloway	147 (1990) 3	351
Dielectrics		
High resolution Raman measurements of the temperature dependence of the phonon line-		
width in lithium formate monohydrate crystals, M. Jordan, H.J. Jodl and M. Maier	147 (1990)	155
Chemical and physical effects during spontaneous relaxation of a network-structure glass,		205
D. Sidebottom and G.P. Johari	147 (1990)	205
Microscopic systems		
Atoms		
Hot atom kinetic theory: changes in average reaction energy, K.D. Knierim	147 (1990)	109
Repulsive ion-atom and ion-ion potentials from charge density overlap integrals,		
C. Nyeland, K.T. Tang and J.P. Toennies	147 (1990)	229
Valence electronic densities and electrostatic potentials in ab initio effective core potential		
procedures, L. Fernandez Pacios	147 (1990)	335
Pure state $Ne^{*(*)}[ J, M\rangle]$ -preparation in a magnetic field: polarization effects in ionizing collisions, J.P.J. Driessen, H.J.L. Megens, M.J. Zonneveld, H.A.J. Senhorst,		
collisions, J.P.J. Driessen, H.J.L. Megens, M.J. Zonneveld, H.A.J. Senhorst, H.C.W. Beijerinck and B.J. Verhaar	147 (1990)	447
11.0. W. Deljermer and D.S. Verhaar	147 (1770)	77/
Molecules (neutral and ionic)		
Transition metal 2p excitation of organometallic compounds studied by electron energy	4.45 (4.000)	
loss spectroscopy, A.P. Hitchcock, A.T. Wen and E. Rühl	147 (1990)	51
Functional counterpoise corrections for the NMR chemical shift in a model dimeric water	147 (1990)	01
system, D.B. Chesnut and C.G. Phung Multiparent configuration interaction calculations of low-lying states of $O_2^{2+}$ , H. Yang,	147 (1990)	91
D.M. Hanson, F.V. Trentini and J.L. Whitten	147 (1990)	115
D.M. Hanson, 1. v. Homan and J.D. William	147 (1770)	113
-diatomic		
Dissociative chemisorption of N <sub>2</sub> on rhenium: dynamics at low impact energies,	147 (1000)	
G.D. Billing, A. Guldberg, N.E. Henriksen and F.Y. Hansen Hartree-Fock limit and configuration interaction calculations of the ion-molecule overlap	147 (1990)	1
amplitude for hydrogen fluoride: comparison with EMS experiments, E.R. Davidson,		
D. Feller, C.M. Boyle, L. Adamowicz, S.A.C. Clark and C.E. Brion	147 (1990)	45
Multiparent configuration interaction calculations of low-lying states of $O_2^{2+}$ , H. Yang,	111 (1330)	
D.M. Hanson, F.V. Trentini and J.L. Whitten	147 (1990)	115
The effect of dynamical correlation on the valence wavefunction of molecules: dressed	,	
complete active space self-consistent field calculations, A. Clotet, J.P. Daudey,		
J.P. Malrieu, J. Rubio and F. Spiegelmann	147 (1990)	293
Theoretical prediction of the radiative lifetimes of the two lowest excited electronic states		
of TeO, S.N. Rai and R.J. Buenker	147 (1990)	327
A theoretical scattering study of oriented NO from a silver surface: effects of surface recoil,	147 (1000)	251
M.R. Hand, X.Y. Chang and S. Holloway	147 (1990)	331

-small polyatomics	
Ab intio MRD CI ground and excited state potential curves for addition of O to H <sub>2</sub> C=CH <sub>2</sub>	
and oxirane formation and decomposition, S. Roszak, R.J. Buenker, P.C. Hariharan and	147 (1000) 13
J.J. Kaufman	147 (1990) 13
An ab initio vibrational study of rotational isomerism in oxalyl fluoride, O=CF-CF=O,	
and acryloyl fluoride, O=CF-CH=CH2, C.W. Bock, Y.N. Panchenko and	
S.V. Krasnoshchiokov	147 (1990) 65
Equilibrium structure and hyperfine parameters of the ethane cation, MB. Huang and	
S. Lunell	147 (1990) 85
Functional counterpoise corrections for the NMR chemical shift in a model dimeric water	
system, D.B. Chesnut and C.G. Phung	147 (1990) 91
On approximately exponential relaxation of polyatomics in bulk systems, W. Forst	147 (1990) 241
Use of the molecular orbital Hessian for self-consistent-field (SCF) wavefunctions,	11. (1550) 211
Y. Yamaguchi, I.L. Alberts, J.D. Goddard and H.F. Schaefer III	147 (1990) 309
	147 (1990) 309
Investigation of laser induced silane/hydrocarbon reactions in the formation of Si and SiC	147 (1000) 200
powders, R. Fantoni, F. Bijnen, S. Piccirillo and S. Enzo	147 (1990) 389
Emission spectra of CO <sub>2</sub> <sup>-</sup> radicals, stabilized in SrCO <sub>3</sub> obtained by thermal decomposition	
of SrC <sub>2</sub> O <sub>4</sub> ·H <sub>2</sub> O, J. Degen, HH. Schmidtke, R. Stoyanova, S. Angelov and M. Atanasov	147 (1990) 415
-aromatics	
The electronic states of the azines. III. Pyrimidine, studied by VUV absorption, near-	
threshold electron energy-loss spectroscopy and ab initio multi-reference configuration	
calculations, M.H. Palmer, I.C. Walker, M.F. Guest and A. Hopkirk	147 (1990) 19
Anharmonic interactions and intramolecular vibrational energy redistribution in anthra-	
cene, S. Rashev	147 (1990) 221
Viscosity effect on the rate of back electron transfer within a short-lived exciplex, E. Vauthey	117 (1770) 221
and D. Phillips	147 (1990) 421
and D. I minps	147 (1990) 421
-polymeric and biological	
Models of pigment-protein interactions in photosynthetic systems: tetraphenylporphyrin	
complexes with polycationic sequential polypeptides. Absorption circular dichroism and	
fluorescence properties, P. Pančoška, M. Urbanová, L. Bednárová, K. Vacek,	
V.Z. Paschenko, S. Vasiliev, P. Maloň and M. Král	147 (1990) 401
Asymmetric photolysis of biomolecules under high-intensity UV laser irradiation,	, ,
D.N. Nikogosyan, Yu.A. Repeyev, E.V. Khoroshilova, I.V. Kryukov, E.V. Khoroshilov	
and A.V. Sharkov	147 (1990) 437
Malandar assessation	
Molecular aggregates	
-dimers	
Functional counterpoise corrections for the NMR chemical shift in a model dimeric water	
system, D.B. Chesnut and C.G. Phung	147 (1990) 91
-clusters	
Field ionizable cesium metal clusters from a foil diffusion source, C. Aman,	
J.B.C. Pettersson and L. Holmlid	147 (1990) 189
	(.,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,

]	Investigation of laser induced silane/hydrocarbon reactions in the formation of Si and SiC powders, R. Fantoni, F. Bijnen, S. Piccirillo and S. Enzo	147 (1990) 389
	-complexes	
	Induced infrared absorption bands of ethylene adsorbed on mordenites: experimental and theoretical studies of electron-donor-acceptor interactions, H. Matsuzawa,	
	H. Yamashita, M. Ito and S. Iwata  Distance dependence of the effective coupling parameters through conjugated ligands of	147 (1990) 77
	the polyene type, C. Joachim, J.P. Launay and S. Woitellier Reinvestigation of the photophysics of the 2-naphthol-amine hydrogen-bonded system. I,	147 (1990) 131
	P.B. Bisht, H.B. Tripathi and D.D. Pant	147 (1990) 173
	Free radicals (including hydronium and muonium)	
	Equilibrium structure and hyperfine parameters of the ethane cation, MB. Huang and	
	S. Lunell	147 (1990) 85
	Flash CIDNP investigation of a cyclic photoreaction, M. Goez	147 (1990) 143
	Magnetic field and magnetic isotope effects in micelles. The kinetics of photochemical re-	
	actions, I.A. Shkrob and V.F. Tarasov	147 (1990) 369
	Ions and charge carriers	
	Surface ionization of organometallic compounds: organic derivatives of main group III-	
	V elements, T. Fujii, K. Kakizaki and H. Ishii	147 (1990) 213
	Repulsive ion-atom and ion-ion potentials from charge density overlap integrals,	
	C. Nyeland, K.T. Tang and J.P. Toennies	147 (1990) 229
	Phenomena	
	Molecular structure	
	Ab intio MRD CI ground and excited state potential curves for addition of O to H <sub>2</sub> C=CH <sub>2</sub> and oxirane formation and decomposition, S. Roszak, R.J. Buenker, P.C. Hariharan and	
	J.J. Kaufman	147 (1990) 13
	Equilibrium structure and hyperfine parameters of the ethane cation, MB. Huang and	
	S. Lunell	147 (1990) 85
	Functional counterpoise corrections for the NMR chemical shift in a model dimeric water	
	system, D.B. Chesnut and C.G. Phung	147 (1990) 91
	Chemical and physical effects during spontaneous relaxation of a network-structure glass,	
	D. Sidebottom and G.P. Johari	147 (1990) 205
	Molecular conformations from ultraviolet photoelectron spectra: substituted anilines,	147 (1000) 047
	J.P. LaFemina, C.B. Duke and W. Rettig	147 (1990) 343
	Manifestation of the Jahn-Teller active vibrations in the vibronic spectra of tetracoordinate Cu <sup>2+</sup> , Ni <sup>2+</sup> and Zn <sup>2+</sup> chlorides, N. Trendafilova, G.St. Nikolov, R. Kellner, H. Mikosch, G. Bauer and G. Bogatchev	147 (1990) 377
	Vibrations and rotations of molecules	
	An ab initio vibrational study of rotational isomerism in oxalyl fluoride, O=CF-CF=O,	
	and acryloyl fluoride, O=CF-CH=CH <sub>2</sub> , C.W. Bock, Y.N. Panchenko and	
	S.V. Krasnoshchiokov	147 (1990) 65
		(/

Induced infrared absorption bands of ethylene adsorbed on mordenites: experimental and theoretical studies of electron-donor-acceptor interactions, H. Matsuzawa, H. Yamashita, M. Ito and S. Iwata	147 (1990) 77
Electronic structure and states	
Ab intio MRD CI ground and excited state potential curves for addition of O to H <sub>2</sub> C=CH <sub>2</sub> and oxirane formation and decomposition, S. Roszak, R.J. Buenker, P.C. Hariharan and J.J. Kaufman	147 (1990) 13
The electronic states of the azines. III. Pyrimidine, studied by VUV absorption, near- threshold electron energy-loss spectroscopy and ab initio multi-reference configuration	
calculations, M.H. Palmer, I.C. Walker, M.F. Guest and A. Hopkirk  Hartree-Fock limit and configuration interaction calculations of the ion-molecule overlap amplitude for hydrogen fluoride: comparison with EMS experiments, E.R. Davidson,	147 (1990) 19
D. Feller, C.M. Boyle, L. Adamowicz, S.A.C. Clark and C.E. Brion  Transition metal 2p excitation of organometallic compounds studied by electron energy	147 (1990) 45
loss spectroscopy, A.P. Hitchcock, A.T. Wen and E. Rühl Multiparent configuration interaction calculations of low-lying states of $\mathrm{O}_2^{2+}$ , H. Yang,	147 (1990) 51
D.M. Hanson, F.V. Trentini and J.L. Whitten  The nuclear quadrupole interaction of <sup>187</sup> W(β <sup>-</sup> ) <sup>187</sup> Re in a 2H-WS <sub>2</sub> single crystal,  P. Mottner and T. Butz	147 (1990) 115
The effect of dynamical correlation on the valence wavefunction of molecules: dressed complete active space self-consistent field calculations, A. Clotet, J.P. Daudey,	147 (1990) 199
J.P. Malrieu, J. Rubio and F. Spiegelmann Use of the molecular orbital Hessian for self-consistent-field (SCF) wavefunctions,	147 (1990) 293
Y. Yamaguchi, I.L. Alberts, J.D. Goddard and H.F. Schaefer III Theoretical prediction of the radiative lifetimes of the two lowest excited electronic states of TeO, S.N. Rai and R.J. Buenker	147 (1990) 309 147 (1990) 327
Valence electronic densities and electrostatic potentials in ab initio effective core potential procedures, L. Fernandez Pacios	147 (1990) 335
Molecular conformations from ultraviolet photoelectron spectra: substituted anilines, J.P. LaFemina, C.B. Duke and W. Rettig  Manifestation of the Jahn-Teller active vibrations in the vibronic spectra of tetracoor-	147 (1990) 343
dinate Cu <sup>2+</sup> , Ni <sup>2+</sup> and Zn <sup>2+</sup> chlorides, N. Trendafilova, G.St. Nikolov, R. Kellner, H. Mikosch, G. Bauer and G. Bogatchev	147 (1990) 377
Emission spectra of CO <sub>2</sub> <sup>-</sup> radicals, stabilized in SrCO <sub>3</sub> obtained by thermal decomposition of SrC <sub>2</sub> O <sub>4</sub> ·H <sub>2</sub> O, J. Degen, HH. Schmidtke, R. Stoyanova, S. Angelov and M. Atanasov Angle-resolved photoelectron study of the group VIB metal hexacarbonyls M(CO) <sub>6</sub>	147 (1990) 415
(M=Cr, Mo, W) from 9 to 30 eV photon energy, B.W. Yates, G.A. von Wald, J.W. Taylor, F.A. Grimm and J.S. Tse	147 (1990) 431
Electric and magnetic properties	
Equilibrium structure and hyperfine parameters of the ethane cation, MB. Huang and S. Lunell	147 (1990) 85
Chemical and physical effects during spontaneous relaxation of a network-structure glass, D. Sidebottom and G.P. Johari	147 (1990) 205
Magnetic field and magnetic isotope effects in micelles. The kinetics of photochemical reactions, I.A. Shkrob and V.F. Tarasov	147 (1990) 369

Spin splittings	
Development and optimization of shaped NMR pulses for the study of coupled spin sys-	
tems, B. Ewing, S.J. Glaser and G.P. Drobny	147 (1990) 121
Theoretical prediction of the radiative lifetimes of the two lowest excited electronic states of TeO, S.N. Rai and R.J. Buenker	147 (1990) 327
Optical activity	
First experimental evidence of circularly polarized X-ray excited optical luminescence (XEOL) from chiral Eu <sup>3+</sup> complexes, C. Gauthier, I. Ascone, J. Goulon, R. Cortes, JM. Barbe and R. Guilard	147 (1990) 165
Models of pigment-protein interactions in photosynthetic systems: tetraphenylporphyrin complexes with polycationic sequential polypeptides. Absorption circular dichroism and fluorescence properties, P. Pančoška, M. Urbanová, L. Bednárová, K. Vacek,	147 (1000) 401
V.Z. Paschenko, S. Vasiliev, P. Maloň and M. Král	147 (1990) 401
Molecular interactions	
Repulsive ion-atom and ion-ion potentials from charge density overlap integrals, C. Nyeland, K.T. Tang and J.P. Toennies	147 (1990) 229
Spectral bandshapes and intensities	
High resolution Raman measurements of the temperature dependence of the phonon linewidth in lithium formate monohydrate crystals, M. Jordan, H.J. Jodl and M. Maier	147 (1990) 155
Coupling of electronic and nuclear motion	
Manifestation of the Jahn-Teller active vibrations in the vibronic spectra of tetracoordinate Cu <sup>2+</sup> , Ni <sup>2+</sup> and Zn <sup>2+</sup> chlorides, N. Trendafilova, G.St. Nikolov, R. Kellner,	
H. Mikosch, G. Bauer and G. Bogatchev	147 (1990) 377
Energy transfer processes	
On approximately exponential relaxation of polyatomics in bulk systems, W. Forst A theoretical scattering study of oriented NO from a silver surface: effects of surface recoil,	147 (1990) 241
M.R. Hand, X.Y. Chang and S. Holloway	147 (1990) 351
Magnetic field and magnetic isotope effects in micelles. The kinetics of photochemical reactions, I.A. Shkrob and V.F. Tarasov	147 (1990) 369
Molecular photophysical processes	
Reinvestigation of the photophysics of the 2-naphthol-amine hydrogen-bonded system. I, P.B. Bisht, H.B. Tripathi and D.D. Pant	147 (1990) 173
Viscosity effect on the rate of back electron transfer within a short-lived exciplex, E. Vauthey	
and D. Phillips  Angle-resolved photoelectron study of the group VIB metal hexacarbonyls M(CO) <sub>6</sub>	147 (1990) 421
(M=Cr, Mo, W) from 9 to 30 eV photon energy, B.W. Yates, G.A. von Wald,	147 (1000) 421
J.W. Taylor, F.A. Grimm and J.S. Tse	147 (1990) 431

## Intramolecular dynamics

-vibrational energy redistribution (including vibrational dissociation)	
High resolution Raman measurements of the temperature dependence of the phonon line-	
width in lithium formate monohydrate crystals, M. Jordan, H.J. Jodl and M. Maier Anharmonic interactions and intramolecular vibrational energy redistribution in anthra-	147 (1990) 155
cene, S. Rashev	147 (1990) 221
Luminescence spectra, yields and lifetimes	
First experimental evidence of circularly polarized X-ray excited optical luminescence	
(XEOL) from chiral Eu <sup>3+</sup> complexes, C. Gauthier, I. Ascone, J. Goulon, R. Cortes,	
JM. Barbe and R. Guilard	147 (1990) 165
Reinvestigation of the photophysics of the 2-naphthol-amine hydrogen-bonded system. I, P.B. Bisht, H.B. Tripathi and D.D. Pant	147 (1990) 173
Emission spectra of CO <sub>2</sub> <sup>-</sup> radicals, stabilized in SrCO <sub>3</sub> obtained by thermal decomposition	147 (1990) 173
of SrC <sub>2</sub> O <sub>4</sub> ·H <sub>2</sub> O <sub>5</sub> J. Degen, HH. Schmidtke, R. Stoyanova, S. Angelov and M. Atanasov	147 (1990) 415
Multiphoton phenomena	
Asymmetric photolysis of biomolecules under high-intensity UV laser irradiation, D.N. Nikogosyan, Yu.A. Repeyev, E.V. Khoroshilova, I.V. Kryukov, E.V. Khoroshilov	
and A.V. Sharkov	147 (1990) 437
Reactions (including dissociation)	
Dissociative chemisorption of N <sub>2</sub> on rhenium: dynamics at low impact energies,	
G.D. Billing, A. Guldberg, N.E. Henriksen and F.Y. Hansen	147 (1990) 1
-gas phase	
Ab intio MRD CI ground and excited state potential curves for addition of O to H <sub>2</sub> C=CH <sub>2</sub> and oxirane formation and decomposition, S. Roszak, R.J. Buenker, P.C. Hariharan and	
J.J. Kaufman	147 (1990) 13
Hot atom kinetic theory: changes in average reaction energy, K.D. Knierim	147 (1990) 109
Investigation of laser induced silane/hydrocarbon reactions in the formation of Si and SiC	
powders, R. Fantoni, F. Bijnen, S. Piccirillo and S. Enzo	147 (1990) 389
-photochemical	
Magnetic field and magnetic isotope effects in micelles. The kinetics of photochemical re-	
actions, I.A. Shkrob and V.F. Tarasov	147 (1990) 369
Asymmetric photolysis of biomolecules under high-intensity UV laser irradiation, D.N. Nikogosyan, Yu.A. Repeyev, E.V. Khoroshilova, I.V. Kryukov, E.V. Khoroshilov	
and A.V. Sharkov	147 (1990) 437
and A. V. Sharavy	147 (1770) 437
Tunnelling	
Distance dependence of the effective coupling parameters through conjugated ligands of	
the polyene type, C. Joachim, J.P. Launay and S. Woitellier	147 (1990) 131
Electron transfer	
Distance dependence of the effective coupling parameters through conjugated ligands of	
the polyene type, C. Joachim, J.P. Launay and S. Woitellier	147 (1990) 131

Flash CIDNP investigation of a cyclic photoreaction, M. Goez	147 (1990) 143
Viscosity effect on the rate of back electron transfer within a short-lived exciplex, E. Vauthey	
and D. Phillips	147 (1990) 421
Ionization (including Rydberg states)	
The electronic states of the azines. III. Pyrimidine, studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration	
calculations, M.H. Palmer, I.C. Walker, M.F. Guest and A. Hopkirk	147 (1990) 19
Field ionizable cesium metal clusters from a foil diffusion source, C. Åman,	147 (1000) 100
J.B.C. Pettersson and L. Holmlid	147 (1990) 189
Surface ionization of organometallic compounds: organic derivatives of main group III- V elements, T. Fujii, K. Kakizaki and H. Ishii	147 (1990) 213
Angle-resolved photoelectron study of the group VIB metal hexacarbonyls M(CO) <sub>6</sub>	147 (1990) 213
(M=Cr, Mo, W) from 9 to 30 eV photon energy, B.W. Yates, G.A. von Wald,	
J.W. Taylor, F.A. Grimm and J.S. Tse	147 (1990) 431
Pure state $Ne^{*(*)}[ J,M\rangle]$ -preparation in a magnetic field: polarization effects in ionizing	(1770) 101
collisions, J.P.J. Driessen, H.J.L. Megens, M.J. Zonneveld, H.A.J. Senhorst,	
H.C.W. Beijerinck and B.J. Verhaar	147 (1990) 447
Molecular motion (including diffusive)	
Chemical and physical effects during spontaneous relaxation of a network-structure glass,	
D. Sidebottom and G.P. Johari	147 (1990) 205
Magnetic field and magnetic isotope effects in micelles. The kinetics of photochemical re-	
actions, I.A. Shkrob and V.F. Tarasov	147 (1990) 369
Surface effects and catalysis	
Surface ionization of organometallic compounds: organic derivatives of main group III-	
V elements, T. Fujii, K. Kakizaki and H. Ishii	147 (1990) 213
A theoretical scattering study of oriented NO from a silver surface: effects of surface recoil,	
M.R. Hand, X.Y. Chang and S. Holloway	147 (1990) 351
Structure of solids and liquids	
Screened dipolar interactions in some molecular crystals, R.W. Munn and M. Hurst	147 (1990) 35
Development and optimization of shaped NMR pulses for the study of coupled spin sys-	
tems, B. Ewing, S.J. Glaser and G.P. Drobny	147 (1990) 121